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DEVELOPMENT OF MOBILE INFRARED SPECTROSCOPY FOR ON-SITE SPECIATION OF ORGANIC WASTES

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ABSTRACT

The stability and performance of three Fourier transform infrared (FT-IR) spectrometers, equipped with either conventional or corner-cube Michelson interferometer, is investigated. Evaluation of instrument stability is based on interferogram subtraction and 100% line interpretation. It is demonstrated that corner-cube retroreflectors compensate for the interferometer optical alignment and eliminate vibrational problems in mobile laboratory. In addition, FT-IR increases the field capacity and provides rapid turnaround time in the identification and classification of hazardous organic wastes.

INTRODUCTION

The mobile unit of the Ontario Ministry of the Environment is equipped with state-of-the-art analytical instrumentation to perform on-site analysis of hazardous wastes for prompt remedial action and solve environmental problems. In order to increase the field capacity in the classification and identification of hazardous organic wastes and to provide rapid turnaround time capability, the unit is investigating the suitability of a Fourier transform infrared (FT-IR) spectrometer for the mobile laboratory. In order to perform a "real world" test we have installed and tested three commercial FT-IR spectrometers in the mobile laboratory during various field investigations. The evaluation was based upon: a) "bouncing test" in which FT-IR spectrometer was shipped to the destination in the mobile laboratory and tested for the stability of the interferometer and basic optical components;

and b) the versatility of each individual data systems and software employed to facilitate the classification and identification of various organic wastes. It is illustrated that infrared spectroscopy, when used concomitantly with appropriate algorithm can fulfill the desired goals.

FT-IR SPECTROMETERS

Three FT-IR spectrometers, namely BOMEM Michelson 100, Digilab FTS-7 and Nicolet 5DX were evaluated. The last two FT-IRs were equipped with a conventional Michelson interferometer and proprietary designed data system for optimized FT-IR spectral data manipulation. The first FT-IR had a corner-cube Michelson interferometer. An IBM PC-AT (or compatible) data station was used to control the spectrometer and to perform the spectral data manipulation. All three spectrometers were equipped with a 1200°K infrared source, triglycine sulfate detector and a 16-bit analog-to-digital converter. Software adjustable gain-ranging was turned off in all three FT-IRs; therefore, stability evaluation performed on these three FT-IR systems was reflecting the nature of a corner-cube and a conventional Michelson interferometer FT-IR.

INTERFEROGRAM SUBTRACTION

The stability and repeatability of an interferometer is best tested using interferogram subtraction approach. It consists of subtracting two consecutive one-scan interferograms. In theory, difference interferogram will reveal the short term stability

problem of the interferometer, i.e., repeatability of the moving mirror drive. Therefore, a residual center burst which maintains the line shape (with either a negative going or a positive going maximum) of the original center burst and with a value <1% of the original center burst is considered to be acceptable. A residual center burst with a derivative line shape and/or a value >2% of the original center burst is an indication of a short term stability problem and should be corrected before proceeding further.

Evaluation performed on the three FT-IRs indicated no signs of such short term stability problem. In addition, values of residual interferogram obtained from the two Michelson interferometers were from 0.2 to 0.8% and was about twice as much when compared to that obtained from the corner-cube interferometer, which ranges from 0.1% to 0.35%.

HUNDRED PERCENT LINE INTERPRETATION

Hundred percent line is used to evaluate a poor mirror drive because it would produce random tilting and perturbs high frequency component more than lower frequency component; thus, result in a 100% line which deviates from the 100% transmittance. In our experiment all three FT-IRs showed no such abnormality. Furthermore, noise level obtained from a single scan, resolution 4 cm^{-1} 100% line spectrum from all three FT-IRs was about 0.18% $\pm$ 0.02% which matched well with that can be generated from a 16-bit analog-to-digital converter. It was noticed that 100% spectrum measured from the corner-cube interferometer, via ratioing single

beam spectra collected before and after the trip, had a deviation of about ± 20% from the 100% transmittance. We were not able to obtain a similar 100% line from the other two FT-IRs. In fact, minor optical adjustment was required to bring the two FT-IRs to the original performing standards.

SPECIATION OF ORGANIC WASTES

Hazardous waste samples normally contain one principal component along with several minor contaminants. Mandatory separation and purification is required to assure the effective use of mass spectrometry. Infrared spectrometry, on the other hand, reveals functional group information of the sample and is not subjected to the prerequisite imposed on the mass spectrometry. In addition, the availability of infrared libraries and structure prediction software make it possible for an infrared spectroscopist to classify and identify most of the incoming organic wastes. All of the above advantages make infrared spectrometry an ideal choice for on-site organic wastes speciation task and offers a fast turnaround time that cannot be matched by any other existing analytical techniques.

CONCLUSIONS

Evaluation performed in the laboratory shows that FT-IR is a valuable tool for on-site organic waste speciation. The corner-cube interferometer FT-IR offers both short term and long term stability for the speciation of organic wastes. The field capacity was increased by at least a factor of 3.